**European Summer School on Multiscale Modeling in CRE – Short Report**

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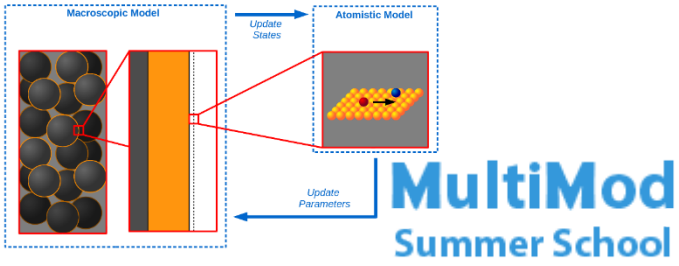


The "European Summer School on Multiscale Modeling in Chemical Reaction Engineering" took place at the Porto Carras Resort in Chalkidiki, Greece, from the 18th to the 22nd of September 2017. Its purpose was to give an overview about the different scales of modeling in chemical reaction engineering - from the atomistic level to the reactor design - and how to bridge these scales in a multiscale modeling approach.

Each day we had some lectures often in combination with associated exercises that provided hands-on experience. On Monday Professor Freund from FAU and Professor Krewer from TUB gave an introduction to multiscale modeling in chemical reaction engineering. One challenge is that the length and time scales spread over several orders of magnitude - of picoseconds and picometers at the active site level to months and meters at the plant level. Hence, for building up a comprehensive multiscale model of a single process bridging all these scales with a minimal loss of information, people from different scientific backgrounds, such as physical chemistry and process engineering, have to communicate with each other and to work together. One has to keep in mind that model predictions are always subjective and that the required accuracy of the model strongly depends on what details of the process are of interest. Professor Voutetakis from CERTH gave a lecture on combining modeling and experiments in pilot catalytic processes. For an optimal process control of pilot plants it is crucial to be able to calculate the required control actions for a future horizon. The challenge is to find the best trajectory to the set point as the direct way to the set point is not always the best. Finally, Professor Kevrekidis from Princeton gave a lecture on the topic of how to find out the variables that strongly influence your system and that should therefore be embedded in the macroscopic model. He presented a computational method which basic idea is to run a microscopic model selectively at single points and subsequently the obtained data is reduced by a Principal Component Analysis (PCA) to unveil significant variables for calculating.

On Tuesday Professor Froudakis from U Crete gave a lecture about *ab-initio quantum* chemistry calculations. By simplifying the Schrödinger equation by reasonable approximations the structure of molecules can be calculated by only using physical constants as an input. Out of these calculations you obtain important information about molecules, such as the binding length or the enthalpy of formation, that are needed as input for microscale modeling like DFT (Density Functional Theory) or Monte-Carlo Simulations. Professor Saeys from U Ghent gave an introduction to DFT-guided construction of microkinetic models. Microkinetic models can be very complex comprising a network of several hundred possible reactions. The functional form of the model is determined by the DFT, whereas the parameters inside the model are derived from experiments. A sensitivity analysis can help to find out which components are sensitive to the kinetics.

On Wednesday the Professor Reuter from the TU Munich held a lecture and an exercise about the basis of kinetic Monte Carlo Simulation: the adsorption of different components at the catalytic

surface and their possible interactions can be studied. In that way the different steps of a microkinetic can be simulated and evaluated as soon as hypothesis about the rate determining step are assumed.

Professor Deutschmann from KIT presented on Thursday the methods for connecting the micro to the macro kinetic. The partial oxidation of $CH_4$ was object of the theoretical explanation of the competition between reaction and diffusion in heterogeneous catalysis. In parallel the process was object of the exercises and the DETCHEM$^{TM}$ package was presented. It was possible to use the program for the calculation from the thermodynamic equilibrium till the macrokinetic for a 2D description of the reactor taking account of the mass and heat transports. It was the only case where the lecture and the exercises were taken at the same time.

In the afternoon the Professor Maestri from the Politecnico di Milano presented through both a lecture and an exercise session the possibility of combining the mikrokinetic modeling with CFD simulation. During the exercise there was the possibility to see how a catalytic monolith can be constructed with the catalyticFOAM tool.

On Friday Professor Dittmeyer from KIT presented how microreactors can be modelled using MatLab® tools. The example of the $CH_4$ steam reforming in a micro membrane-reactor was explained and the lecture aimed to give instruments for the passage from the micro to reactor scale. Scope of this simulation was also to get the best configuration of the process in terms of catalyst loading, feed flow rate, temperature and pressure in order to get the highest conversion and hydrogen recovery.

On Thursday evening a poster session took place. All participants presented a poster illustrating their research project. In a comfortable atmosphere it was possible to inform oneself about the research project that other groups in the same field are currently working on. A lot of fruitful discussions arose and some opportunities for future collaborations were opening up.

The communal meals and coffee breaks promoted the discussion between the participants. One could expand one's own network and one could get new impulses for one's own work through the discussions and exchange of ideas. The well-organized framework programme contributed to get in touch with the Greece culture by the help of wine testing event in a new generation winery and during the gala dinner with traditional dances of several regions of Greece. All this made the stay in Greece successful and instructive. All the participants got a good overview of the different approaches of the multiscale modeling for heterogeneous catalysis. The lectures and the exercises offered the opportunity to go in deep and expand the knowledge from the different points of view.